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ON THE CALCULATION OF SOME ATOMIC INTEGRALS CONTAINING FUNCTIONS OF r_{12}, r_{13} AND r_{23}

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Quantum Chemistry Group
For Research in Atomic, Molecular and Solid-State Theory
Uppsala University, Uppsala, Sweden

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† This work was concluded while the authors were members of the Quantum Theory Project at the University of Florida

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ABSTRACT

Different forms of correlated atomic wave functions and their implications on the integrals occurring in calculations of variational solution to Schrödinger's equation are briefly discussed. A scheme for computing the integral

$$\int f_1(r_1) f_2(r_2) f_3(r_3)\, g_1(r_{12})\, g_2(r_{23})\, g_3(r_{31})\, (dv)$$

is described and applied to the case $g_i(r_{ij}) = r_{ij}^{k}$

I. INTRODUCTION

In atomic and molecular theory several variational solutions to the Schroedinger equation have been obtained for a variety of small systems using trial wave functions of a varying degree of complexity. The different methods of calculating variational solutions are commonly classified according to the analytical form of trial wave function used.[1] The method of so-called correlated wave functions, i.e. functions that depend explicitly on the interelectronic distances $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ was first introduced by Hylleraas.[2] The method has later been used in numerous applications on small systems, predominantly two-electron systems. One of the

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1) P.O. Löwdin, Adv. Chem Phys. 2 , 207 (Interscience Publ. L Prigogine,Ed. New York, 1959)

2) E.A. Hylleraas, Z. Phys. 54 , 347 (1929)

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merits of the method is that it gives good results and yet can give wave functions in an attractively condensed form. It seems to be fairly difficult, however, to generalize the method to systems with more than two electrons. One of the main obstacles is that considerable difficulties are met in calculating the integrals with several interelectronic distances in the integrand. Recently some progress has been made in generalizing the method of correlated wave functions to many electron atoms,[3] but still an accurate calculation of the integrals containing functions of r_{ij} seems to be an unsolved problem in its full generality.

Several different methods have been suggested[4-8] how to

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3) L. Szasz, Phys. Rev. 126 , 169 (1962)

4) H.M. James and A.S. Coolidge, Phys. Rev. 49 688 (1936)

5) V. Fock, M. Vesselov and M. Petrashen, J. Explo. Theoret. Phys. (USSR), 10 , 723 (1940)

6) P. Walsh and S. Borowitz, Phys. Rev. 115 , 1206 (1959)

7) L. Szasz, J.C.P. 35 , 1072, (1961)

8) J.L. Calais and P.O. Löwdin , J. Mol. Spec. 8, 203 (1962)

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calculate such integrals and the purpose of this note is to describe a simple scheme for computing certain atomic integrals that have an explicit dependence of inter-electronic distances in the integrand.

II. FORMULATION OF THE PROBLEM

Without using carefully designed forms of the correlated wave functions we would have to evaluate integrals of a considerable complexity. But if we e.g. use trial wave functions of the form

(1) $\Psi \equiv g(r_{12}, r_{13}, \dots r_{N-1,N}; r_1, r_2, \dots r_N)\, \Phi(\underline{x}_1, \underline{x}_2, \dots \underline{x}_N)$,

where the analytical form of g and Φ are restricted to certain important simple cases, it is possible to make progress in the calculations of the occurring integrals. Φ may be an antisymmetrized product of suitably chosen spin orbitals or a superposition of such products, and g a nodeless function, symmetrical with respect to permutations of the electronic coordinates.[1),9)]

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9) L. Redei and P.O. Löwdin, Phys. Rev. 114 , 752 (1952)

$\chi_i = \{\underline{r}_i, \xi_i\}$ is here a combined space-spin variable, such that $\underline{r}_i$ is the position vector of the electron i with respect to the nucleus and ξ_i a spin variable. Slightly more general trial functions of the same type have also been suggested with g not necessarily a function of all the interelectronic distances.[3)]

(2) $\Psi \equiv \mathcal{A} g(r_{12}, r_{13}, \dots r_{n-1,n}; r_1, r_2 \dots r_n)\, \Phi(\chi_1, \chi_2, \dots \chi_N)$,

where $2 \leq n \leq N$ and $\mathcal{A}$ is the antisymmetrizer in N-particle space. The correlation factor g has often been chosen as a polynomial of r_i, r_j and r_{ij} with suitable adjustable parameters, but also other simple analytical forms have been used.[6),10)]

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10) P. Walsh and S. Borowitz, Phys. Rev. 119 , 1274 (1960)

If we keep in mind all these and other common restrictions on the correlated wave functions used so far in atomic calculation it may be general enough to start out by treating an integral of the form

(3) $$\int f_1(\vec{r}_1) f_2(\vec{r}_2) \dots f_N(\vec{r}_N)\, g_1(r_{12})\, g_2(r_{23}) \dots g_k(r_{m,m-1})\, (dv)$$

This may factorize into integrals of lower dimensions where the integration variables are coupled through the interelectronic distances. The simplest non-trivial form of such a factor would be

$$K(a\,l_1 m_1, b\,l_2 m_2, c\,l_3 m_3 \mid d\,l_4 m_4, e\,l_5 m_5, f\,l_6 m_6) \equiv$$

(4) $$\int a^*(\vec{r}_1) Y^*_{l_1 m_1}(1)\, b^*(\vec{r}_2) Y^*_{l_2 m_2}(2)\, c^*(\vec{r}_3) Y^*_{l_3 m_3}(3)$$

$$\times d(\vec{r}_1) Y_{l_4 m_4}(1)\, e(\vec{r}_2) Y_{l_5 m_5}(2)\, f(\vec{r}_3) Y_{l_6 m_6}(3)\, g_1(r_{12}) g_2(r_{23}) g_3(r_{31})\, (dv),$$

where we have used the orbital form $r(r)\, Y_{l m_l}(\theta, \phi)$ explicitly. Here Y_{lm} is a spherical harmonic as defined e.g. in Edmonds' book.[11]

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11) A.R. Edmonds, "Angular Momentum in Quantum Mechanics", (Princeton University Press, 1957)

If we now expand a product of spherical harmonics according to the formula

$$Y^{*}_{l_1 m_1} Y_{l_4 m_4} = (-1)^{m_1} Y_{l_1 -m_1} Y_{l_4 m_4} =$$

(5)
$$(-1)^{m_4} \sum_{n=|l_1-l_4|}^{l_1+l_4} \left\{ \frac{(2l_1+1)(2l_4+1)(2n+1)}{4\pi} \right\}^{1/2} \times \begin{pmatrix} l_1 & l_4 & n \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_4 & n \\ -m_1 & m_4 & -m \end{pmatrix} Y^{\dagger}_{n m},$$

where $m = m_1 - m_4$, we can write K as a sum of integrals

(6)
$$I^{t u v}_{l i j} = (4\pi)^{-3/2} \int f_1(r_1) f_2(r_2) f_3(r_3) Y_{l t}(1) Y_{i u}(2) Y_{j v}(3) \times g_1(r_{12}) g_2(r_{23}) g_3(r_{31}) (dv).$$

For instance $K(a00, b10, c10 | d00, e10, f10)$ will become a linear combination of I^{000}_{000}, I^{000}_{010}, I^{000}_{002} and I^{000}_{012}. Here $a^{*}(r_1) d(r_1) b^{*}(r_2) e(r_2) c^{*}(r_3) f(r_3) \equiv f_1(r_1) f_2(r_2) f_3(r_3)$ and $t = m_1 - m_4$, $u = m_2 - m_5$, $v = m_3 - m_6$.

The Wigner 3-j symbols are defined in reference 11. Further we can write[12]

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12) P.O. Löwdin, "A Theoretical Investigation into Some Properties of Ionic Crystals", Thesis, Uppsala, 1948 (Almqvist and Wiksell).

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† Compare formula (4.6.5) in reference 11, and specific formulas in reference 15.

$$(7)\qquad q_i(r_{ij}) = \sum_{n=0}^{\infty} \alpha_n(r_i, r_j | q_i)\, P_n(\cos\theta_{ij}),$$

where $r_{ij}^2 = r_i^2 + r_j^2 - 2 r_i r_j \cos\theta_{ij}$, P_n is the Legendre polynomial of degree n and

$$(8)\qquad \alpha_n(r_i, r_j | q_i) = \frac{2n+1}{2} \int q_i(r_{ij})\, P_n(\cos\theta_{ij}) \sin\theta_{ij}\, d\theta_{ij}.$$

Equation (7) together with the addition theorem,

$$(9)\qquad P_n(\cos\theta_{ij}) = 4\pi(2n+1)^{-1} \sum_{m=-n}^{n} Y_{nm}^*(\theta_i, \phi_i) Y_{nm}(\theta_j, \phi_j)$$

then give

$$(10)\qquad I_{hij}^{tuv} = \sum_{k,l,m} B_{klm}^{(hk|iu|jv)}\, U_{klm}^{(q_1, q_3, q_2)}$$

where

$$(10a)\qquad U_{klm}^{(q_1,q_3,q_2)} = \{(2k+1)(2l+1)(2m+1)\}^{-1} \times \int_0^\infty \int_0^\infty \int_0^\infty f_1(r_1) f_2(r_2) f_3(r_3) \alpha_k(r_1, r_2 | q_1)\, \alpha_l(r_3, r_1 | q_3) \times \alpha_m(r_2, r_3 | q_2)\, r_1^2 r_2^2 r_3^2\, dr_1\, dr_2\, dr_3$$

and

$$B_{klm}(kl|iu|jv) = \sum_{s=-k}^{k} \sum_{\tau=-l}^{l} \sum_{\mu=-m}^{m} (4\pi)^{3/2} \cdot$$

$$\times \int_0^{\pi} \sin\vartheta_1^{\nu}\, d\vartheta_1^{\nu} \int_0^{2\pi} d\varphi_1\, Y^{*}_{k,s}(1)\, Y_{i,\tau}(1)\, Y_{k,s}(1)$$

(10b)

$$\times \int_0^{\pi} \sin\vartheta_2^{\nu}\, d\vartheta_2^{\nu} \int_0^{2\pi} d\varphi_2\, Y^{*}_{k,\tau}(2)\, Y_{m,\tau}(2)\, Y_{i,u}(2)$$

$$\times \int_0^{\pi} \sin\vartheta_3^{\nu}\, d\vartheta_3^{\nu} \int_0^{2\pi} d\varphi_2\, Y^{*}_{m,\tau}(3)\, Y_{k,s}(3)\, Y_{j,v}(3) .$$

By change of integration variable $\vartheta_{ij}^{\nu} \longrightarrow R_i$, where $\cos\vartheta_{ij}^{\nu} = \frac{r_i^2 + r_j^2 - R_i^2}{2 r_i r_j}$, we get from equation (8)

$$(11)\quad \alpha_k(r_i, r_j | q_i) = \frac{2k+1}{2 r_i r_j} \int_{|r_i - r_j|}^{r_i + r_j} q_i(R_i)\, P_k\left(\frac{r_i^2 + r_j^2 - R_i^2}{2 r_i r_j}\right)$$

Depending on the analytical form of the functions $q_i(R)$, we can now proceed in different ways. We can e.g. calculate the $\alpha_k(r_i, r_j | q_i)$ by using the "Q-polynomials" of Löwdin.[13] This

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13) P.O. Löwdin, Adv. in Phys. 5 ,1 (1956); "Quantum Theory of Cohesive Properties of Solids." p.98

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means that we can use the well-known explicit expression for the Legendre polynomials and write

$$(12)\quad \alpha_k(r_i, r_j | q_i) = (2k+1)(2 r_i r_j)^{-k-1} \sum_{s=0}^{k} Q_{k,s}(r_i, r_j) \int_{|r_i - r_j|}^{r_i + r_j} q_i(R_i)\, R_i^{2s+1}\, dR_i$$

Here $Q_{k,s}(r_i, r_j)$ is a homogeneous polynomial in r_i^2 and r_j^2

of degree $(k-s)$. Recursion formulas for the Q's are given in reference 13. The expressions we get for $\alpha_k(r_i, r_j \mid q_i)$ in this way may be tedious and lengthy to work with but are in principle not complicated.

To be specific we have chosen to treat, in the following, the case when q in expressions (1) and (2) is a polynomial in r_i, r_j and r_{ij}. Without loss of generality we can then choose the functions q_i in the integrals (3) and (4) to simply be the powers of the interelectronic distances. From equations (11) and (10a) we get

$$U_{klm}(\lambda,\mu,\nu) = 2^{-3}\int_0^\infty dr_1 \int_0^\infty dr_2 \int_0^\infty dr_3\, f_1(r_1) f_2(r_2) f_3(r_3)$$

$$\times \int_{|r_1-r_2|}^{r_1+r_2} P_k(X_{12}) R_1^{\lambda+1}\, dR_1 \int_{|r_3-r_1|}^{r_3+r_1} P_l(X_{13}) R_3^{\mu+1}\, dR_3 \tag{13}$$

$$\times \int_{|r_2-r_3|}^{r_2+r_3} P_m(X_{23}) R_2^{\nu+1}\, dR_2 ,$$

where $X_{ij} = \dfrac{r_i^2 + r_j^2 - R_i^2}{2 r_i r_j}$. It is now in general necessary to distinguish between the regions $r_i > r_j$ and $r_i < r_j$. This splits U_{klm} into six integrals with different order relations between the integration variables, i.e.

$$\begin{aligned} U_{klm}(\lambda,\mu,\nu) = 2^{-3}\Big\{ &\int_0^\infty f_1(x)\int_x^\infty f_2(y)\int_y^\infty f_3(z) F_{k\lambda}(y>x) F_{l\mu}(z>x) F_{m\nu}(z>y)\, dz\, dy\, dx \\ &+ \int_0^\infty f_2(y)\int_y^\infty f_1(x)\int_x^\infty f_3(z) F_{k\lambda}(x>y) F_{l\mu}(z>x) F_{m\nu}(z>y)\, dz\, dx\, dy \\ &+ \int_0^\infty f_3(z)\int_z^\infty f_2(y)\int_y^\infty f_1(x) F_{k\lambda}(x>y) F_{l\mu}(x>z) F_{m\nu}(y>z)\, dx\, dy\, dz \\ &+ \int_0^\infty f_1(x)\int_x^\infty f_3(z)\int_z^\infty f_2(y) F_{k\lambda}(y>x) F_{l\mu}(z>x) F_{m\nu}(y>z)\, dy\, dz\, dx \\ &+ \int_0^\infty f_2(y)\int_y^\infty f_3(z)\int_z^\infty f_1(x) F_{k\lambda}(x>y) F_{l\mu}(x>z) F_{m\nu}(z>y)\, dx\, dz\, dy \end{aligned} \tag{14}$$

$$+\int_0^\infty f_3(z)\int_z^\infty f_1(x)\int_x^\infty f_2(y)\,F_{k\lambda}(y>x)F_{l\mu}(x>z)F_{m\nu}(y>z)\,dy\,dx\,dz\Big\}.$$

Here

(15a) $$F_{lk}(x>y) = xy\,k(2l+1)^{-1}\left[F_{l+1,k-2}(x>y) - F_{l-1,k-2}(x>y)\right]$$

for $k \geq 1$,

(15b) $$F_{0k}(x>y) = \frac{2}{k+2}\sum_{i=0}^{\left[\frac{k+1}{2}\right]}\binom{k+2}{2i+1}x^{k-2i}y^{2i},$$

where $\left[\frac{k+1}{2}\right]$ = integer part of $\frac{k+1}{2}$, and

(15c) $$F_{l,2m}(x>y) = 0 \quad \text{for } l \geq m+1,$$

(15d) $$F_{l,-1}(x>y) = (2l+1)^{-1}\cdot 2\cdot y^{l+1}x^{-l}$$

Equation (15c) shows that if one of λ, μ and ν is an even number, one of the three infinite summations in equation (10) is reduced to a sum over a finite number of terms.

In order to proceed further with calculation of $U_{k_1}(\lambda_{m_2}\mu\nu)$ we have to be more specific about the form of the radial part of the orbitals. We are in the following going to limit the discussion to orbitals of the form

(16) $$n(r) = \exp\{-ar\}r^n$$

where $n \geq 0$ is an integer. This allows us to include in our treatment radial parts expressed as hydrogen-like functions, Laguerre functions[1] and linear combinations of Slater or Dirichlet functions.[14]

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14) G.G. Hall, Rep. on Progr. in Phys. Vol XXII (1959) p.11

In these cases the U_{klm} from equation (14) that we want to calculate would be superpositions of the $U_{klm}^{(\lambda,\mu,\nu)}$ we get from using the specific form in equation (16) as radial parts.

We now turn to the problem of calculating in coefficients $B_{klm}^{(kl|iu|jv)}$ defined in equation (10b). Here we have to integrate over products of three spherical harmonics. In order to get a non-vanishing contribution from an integral

$$\int_0^{\pi} \sin\vartheta d\vartheta \int_0^{2\pi} d\varphi\, Y_{l_1 m_1}^{*}\, Y_{l_2 m_2}\, Y_{l_3 m_3}$$

it is well known that the following relations have to be fulfilled

$$m_1 = m_2 + m_3 \,, \quad l_1 + l_2 + l_3 = 2n \qquad (n = 0, 1, 2, \dots)$$

$$l_1 + l_3 \geq l_2 \geq |l_1 - l_3| \quad \text{and} \quad l_1 + l_2 \geq l_3 \,.$$

These restrictions give among other things that

$$B_{klm}(kl|iu|jv) = (4\pi)^{3/2} \sum_{\rho = \max\{-k,-(l-l),-(m+\nu)\}}^{\min\{k,\,l+l,\,m-\nu\}}$$

$$\times \int_0^{\pi} \sin\vartheta_1 d\vartheta_1 \int_0^{2\pi} d\varphi_1\, Y_{k,\rho}^{*}(1)\, Y_{l,\rho-l}^{(1)}\, Y_{k,l}(1) \tag{17}$$

$$\times \int_0^{\pi} \sin\vartheta_2 d\vartheta_2 \int_0^{2\pi} d\varphi_2\, Y_{l,\rho-l}^{*(2)}\, Y_{m,\rho+\nu}^{(2)}\, Y_{i,u}^{(2)}$$

$$\times \int_0^{\pi} \sin\vartheta_3 d\vartheta_3 \int_0^{2\pi} d\varphi_3\, Y_{m,\rho+\nu}^{*(3)}\, Y_{k,\rho}^{(3)}\, Y_{j,\nu}^{(3)}$$

and that $B_{klm}(kl|iu|jv) = 0$ if $l + u + \nu \neq 0$ or $k + i + j \neq 2n$, $(n = 0, 1, 2 \dots)$. Schweinler[15] has given useful explicit formulas for expanding products of spherical harmonics of the same argument in spherical harmonics. Formulas of that type are feasable to use in calculation of the integrals in (17).

15) H.C. Schweindler, Quarterly Progress Report, M.I.T., Solid State and Molecular Theory Group, January 15 (1954) p.51

III. FORMULAS FOR CALCULATION

In the numerical evaluation we have extensively used a set of three auxiliary functions[4] defined as

$$\text{(a)} \quad A(\alpha|i) = \int_0^\infty e^{-\alpha x} x^i \, dx$$

$$\text{(18)} \quad \text{(b)} \quad V(\alpha,\beta|m,n) = \int_0^\infty e^{-\alpha x} x^m \, dx \int_x^\infty e^{-\beta y} y^n \, dy$$

$$\text{(c)} \quad W(\alpha,\beta,\gamma|p,q,t) = \int_0^\infty e^{-\alpha x} x^p \, dx \int_x^\infty e^{-\beta y} y^q \, dy \int_y^\infty e^{-\gamma z} z^t \, dz .$$

We will first discuss the "spherically symmetric case" $I^{\circ\circ\circ}_{\circ\circ\circ}$. This we hope will show the main idea of the method and the generalization to other cases is straightforward. $B_{k\ell m}$ in equation (10b) will then reduce to

$$\text{(19)} \quad B_{k\ell m}(00|00|00) = \delta_{k\ell}\,\delta_{\ell m}(2k+1).$$

This together with the restriction on the form of orbitals used, as expressed in equation (16) gives

$$\text{(20)} \quad I(\alpha,\beta,\gamma|pqs|\lambda\mu\nu) = \sum_{k=0}^{\infty} (2k+1)\, U_{kkk}(\lambda,\mu,\nu)$$

where $U_{kkk}(\lambda,\mu,\nu)$ is defined as in equation (13) with $f_1(x) = e^{-\alpha x} x^p$, $f_2(y) = e^{-\beta y} y^q$ and $f_3(z) = e^{-\gamma z} z^s$. It should be noted that we have not normalized the orbitals.

The integrals $I(\alpha,\beta,\gamma|pqs|\lambda\mu\nu)$ can now be expressed in the auxiliary functions A, V and W. We have e.g.

$$I(\alpha,\beta,\gamma|p\,q\,s|\lambda\,0\,0) = A(\gamma|s+2)\,\{\lambda+2\}^{-1}$$

(21a)
$$\times \sum_{i=0}^{\left[\frac{\lambda+1}{2}\right]} \binom{\lambda+2}{2i+1} \left[V(\alpha\beta|p+2+2i,\, q+\lambda+2-2i) + V(\beta\alpha|q+2+2i,\, p+\lambda+2-2i)\right]$$

$$I(\alpha\beta\gamma|pqs|\lambda\,\mu\,0) = \{(\lambda+2)(\mu+2)\}^{-1} \times \sum_{i=0}^{\left[\frac{\lambda+1}{2}\right]} \sum_{j=0}^{\left[\frac{\mu+1}{2}\right]} \binom{\lambda+2}{2i+1}\binom{\mu+2}{2j+1}$$

$$\times \left[W(\alpha\beta\gamma|p+2+2i+2j,\, q+2+\lambda-2i,\, s+2+\mu-2j) + W(\beta\alpha\gamma|q+2+2i,\, p+2+\lambda-2i+2j,\, s+2+\mu-2j)\right.$$

(21b)
$$+W(\gamma\beta\alpha|s+2+2j,\, q+2+2i,\, p+2+\lambda+\mu-2i-2j) + W(\alpha\gamma\beta|p+2+2i+2j,\, s+2+\mu-2j,\, q+2+\lambda-2i)$$

$$\left.+W(\beta\gamma\alpha|q+2+2i,\, s+2+2j,\, p+2+\lambda+\mu-2i-2j) + W(\gamma\alpha\beta|s+2+2j,\, p+2+\mu-2j+2i,\, q+2+\lambda-2i)\right]$$

and

$$I(\alpha\beta\gamma|pqs|-1\,-1\,-1) = \sum_{k=0}^{\omega} (2k+1)^{-2}$$

(22)
$$\times \left[W(\alpha\beta\gamma|p+2+2k,\, q+1,\, s-2k) + W(\beta\alpha\gamma|q+2+2k,\, p+1,\, s-2k)\right.$$

$$+W(\gamma\beta\alpha|s+2+2k,\, q+1,\, p-2k) + W(\alpha\gamma\beta|p+2+2k,\, s+1,\, q-2k)$$

$$\left.+W(\beta\gamma\alpha|q+2+2k,\, s+1,\, p-2k) + W(\gamma\alpha\beta|s+2+2k,\, p+1,\, q-2k)\right].$$

Both (21a) and (21b) represent many integrals of interest in atomic theory. In particular (21a) for $\lambda=-1$ and $A(\gamma|s+2)$ replaced by 1 can be used for calculating the ordinary two-electron repulsion integrals for spherically symmetric functions. The integral in equation (22) is the simplest of the $I(\alpha\beta\gamma|pqs|\lambda\mu\nu)$'s that requires an infinite sum of W's. In connection with (21a) and (21b) we should

also note the trivial but useful relations like

$$I(\alpha\rho\gamma|pqs|\lambda\mu\nu) = I(\beta\alpha\gamma|qps|\lambda\nu\mu) \quad \text{a.s.o.}$$

For certain restrictions on the form of the correlated wave function used,[16] the most complicated integrals bound to occur would be possible to express as linear combinations of $I^{\lambda\mu\nu}_{i,j}(\alpha\rho\gamma|pqs|\lambda\mu-1)$

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16) I. Szasz, Quarterly Progress Report M.I.T. Solid State and Molecular Theory Group, July 15, 1962

To show how such an integral can be calculated we are in section V and in the Appendix discussing in particular

$$\begin{aligned}
&I^{\infty\infty}_{\infty\infty}(\alpha\rho\gamma|pqs|1\,1\,-1) = \\
&= \tfrac{1}{9}\left[W(\alpha\rho\gamma|p+6,q+1,s)+W(\rho\alpha\gamma|q+4,p+3,s)+W(\gamma\rho\alpha|s+4,q+3,p)\right. \\
&\quad \left.+W(\alpha\gamma\rho|p+6,s+1,q)+W(\rho\gamma\alpha|q+4,s+3,p)+W(\gamma\alpha\rho|s+4,p+3,q)\right] \\
&\quad +\sum_{k=1}^{\infty}(2k+1)^{-2}\Big[(2k+3)^{-2}\Big\{W(\alpha\rho\gamma|p+6+2k,q+1,s-2k)+W(\rho\alpha\gamma|q+4+2k,p+3,s-2k) \\
&\qquad +W(\gamma\rho\alpha|s+4+2k,q+3,p-2k)+W(\alpha\gamma\rho|p+6+2k,s+1,q-2k) \\
&\qquad +W(\rho\gamma\alpha|q+4+2k,s+3,p-2k)+W(\gamma\alpha\rho|s+4+2k,p+3,q-2k)\Big\} \\
&\quad -(2k+3)^{-1}(2k-1)^{-1}\Big\{W(\alpha\rho\gamma|p+4+2k,q+1,s+2-2k)+W(\rho\alpha\gamma|q+4+2k,p+1,s+2-2k) \\
&\qquad W(\gamma\rho\alpha|s+2+2k,q+3,p+2-2k)+W(\alpha\gamma\rho|p+4+2k,s+3,q-2k) \\
&\qquad W(\rho\gamma\alpha|q+4+2k,s+1,p+2-2k)+W(\gamma\alpha\rho|s+2+2k,p+5,q-2k)\Big\}
\end{aligned} \tag{23}$$

$$- (2k+3)^{-1}(2k-1)^{-1}\left\{W(\alpha\beta\gamma|p+4+2k, q+3, s-2k)+W(\beta\alpha\gamma|q+2+2k, p+5, s-2k)\right.$$
$$+ W(\gamma\beta\alpha|s+4+2k, q+1, p+2-2k)+W(\alpha\gamma\beta|p+4+2k, s+1, q+2-2k)$$
$$\left.+ W(\beta\gamma\alpha|q+2+2k, s+3, p+2-2k)+W(\gamma\alpha\beta|s+4+2k, p+1, q+2-2k)\right\}$$
$$+ (2k-1)^{-2}\left\{W(\alpha\beta\gamma|p+2+2k, q+3, s+2-2k)+W(\beta\alpha\gamma|q+2+2k, p+3, s+2-2k)\right.$$
$$+ W(\gamma\beta\alpha|s+2+2k, q+1, p+4-2k)+W(\alpha\gamma\beta|p+2+2k, s+3, q+2-2k)$$
$$\left.+W(\beta\gamma\alpha|q+2+2k, s+1, p+4-2k)+W(\gamma\alpha\beta|s+2+2k, p+3, q+2-2k)\right\}\Big].$$

All these formulas do not tell very much about the method unless we also describe how to calculate the A's, V's, and W's and investigate the convergence of the infinite sums. This will be done in sections IV and V.

If at least one of k, i and j in equation (10b) is different from zero we will get more complex situations. For example $k=0$, $i=1$, $j=1$ give $B_{k,k,k+1}^{(00|10|10)}=k+1$ and $B_{k,k,k-1}^{(00|10|10)}=k$ as the only nonvanishing coefficients. It is, however, also for a general $I_{k,i,j}^{\alpha\beta\gamma}$, a straight forward procedure to express it in terms of A's, V's and W's, by going back to formula (14). This means that although we in sections IV and V are practically treating the spherically symmetric case, I_{000}^{000}, methods and results from there are with very few exceptions directly applicable to the general case $I_{k,i,j}^{\alpha\beta\gamma}$.

IV. COMPUTATIONAL SCHEME

In calculating a particular $W(\alpha\beta\gamma|fgh)$, we have to distinguish between two cases, $h \geq 0$ and $h < 0$.

1. When $h \geq 0$ the calculation is set up in three steps.

(i) First we form a table of all $A(\alpha+\beta+\gamma|n)$ for $n = f, f+1, \ldots f+g+h$, using the relation

$$A(\alpha+\beta+\gamma|n) = n\,A(\alpha+\beta+\gamma|0)\,A(\alpha+\beta+\gamma|n-1) \tag{24}$$

where $A(\alpha+\beta+\gamma|0) = (\alpha+\beta+\gamma)^{-1}$ and $n \geq 1$.

(ii) From this table we can then construct a table of $V(\alpha,\beta+\gamma|f,k)$ for $k = g, g+1, \ldots g+h$, using the formula

$$V(\alpha,\beta+\gamma|f,k) = (\beta+\gamma)^{-1}\{A(\alpha+\beta+\gamma|f+k) + kV(\alpha,\beta+\gamma|f,k-1)\} \tag{25}$$

which is valid for $f \geq 0$ and $f+k \geq 0$.

(iii) The final step is now to use the V's to calculate the $W(\alpha,\beta,\gamma|f,g,h)$ of interest. This can be done with the recurrence relation

$$W(\alpha\beta\gamma|fgl) = \gamma^{-1}\{V(\alpha,\beta+\gamma|f,g+l) + lW(\alpha\beta\gamma|f,g,l-1) \tag{26}$$

for l from 0 to h. (26) is not valid unless $f \geq 0$, $f+g \geq 0$, and $f+g+h \geq -1$.

2. In the integrals $I^{\alpha\beta\gamma}_{\delta\varepsilon\zeta}$ that are expressed as infinite sums like those in equations (22) and (23) we need in addition to calculate $W(\alpha\beta\gamma|\delta\varepsilon\zeta\eta)$ for $\eta < 0$. This can not conveniently be done with (24)-(26), partly because it is a tedious procedure to find all the "starting values" $V(\alpha,\beta+\gamma|\delta,-1)$ and $W(\alpha\beta\gamma|\delta\varepsilon-1)$ that are necessary, and partly due to the fact that these recurrence relations will in this case not be numerically stable, i.e. loss of significant figures is bound to occur. In this case $(\eta<0)$ we use the formula

$$(27)\qquad W(\alpha\beta\gamma|\delta\varepsilon\zeta\eta) = \sum_{\mu=1}^{M} \frac{\alpha^{\mu-1}\,\delta!}{(\delta+\mu)!}\, V(\alpha+\beta,\gamma|\delta+\varepsilon+\zeta+\mu,\eta)$$

where for $\mu = M$

$$(28)\qquad V(\alpha+\beta,\gamma|\delta+\varepsilon+\zeta+M,\eta) = \sum_{\nu=1}^{N} \frac{(\alpha+\beta)^{\nu-1}(\delta+\varepsilon+\zeta+M)!}{(\delta+\varepsilon+\zeta+M+\nu)!}\, A(\alpha+\beta+\gamma|\delta+\varepsilon+\zeta+\eta+M+\nu)$$

and for $\mu = M-1,\ldots 1$

$$(29)\qquad V(\alpha+\beta,\gamma|\delta+\varepsilon+\zeta+\mu,\eta) = \frac{1}{\delta+\varepsilon+\zeta+\mu+1}\{(\alpha+\beta)V(\alpha+\beta,\gamma|\delta+\varepsilon+\zeta+\mu+1,\eta) + A(\alpha\beta+\gamma|\delta+\varepsilon+\zeta+\eta+\mu+$$

M and N are in principle infinite, but in actual calculations they are of course assigned finite values. In order to avoid very large and very small quantities these formulas have been combined to the following computational scheme:

$$(30)\qquad W(\alpha\beta\gamma|\delta\varepsilon\zeta\eta) = W_0\{\Sigma_0 \sum_{\mu=1}^{M} x_\mu + \sum_{\mu=2}^{M} y_\mu\}$$

where $$W_0 = \frac{A(\alpha+\beta+\gamma|\delta+\varepsilon+\zeta+1)}{(\delta+1)(\alpha+\beta+\gamma)},$$

and $$\Sigma_0 = \left(\frac{\alpha+\beta}{\alpha+\beta+\gamma}\right)^{M-1} \cdot \frac{(\delta+1)!\,(\delta+\varepsilon+\zeta+M)!}{(\delta+\varepsilon+\zeta+1)!\,(\delta+\varepsilon+M)!} \cdot \frac{\alpha+\beta+\gamma}{\alpha} \cdot \sum_{\nu=1}^{N} S_\nu$$

with $S_\nu = \frac{(\alpha+\beta)}{(\alpha+\beta+\gamma)} \frac{(f+g+h+M+\nu)}{(f+g+M+\nu)} \cdot S_{\nu-1}$ and $S_0 = 1$,

$X_\mu = \frac{\alpha}{(\alpha+\beta)} \cdot \frac{(f+g+\mu)}{(f+\mu)} X_{\mu-1}$ and $X_0 = 1$,

$y_\mu = \frac{(f+g+h+\mu)}{(f+g+\mu)} \left\{ Z_{\mu-1} + \frac{(\alpha+\beta)}{(\alpha+\beta+\gamma)} \cdot y_{\mu-1} \right\}$ with $y_1 = 0$

and $Z_\mu = \frac{\alpha}{(\alpha+\beta+\gamma)} \frac{(f+g+h+\mu)}{(f+\mu)} Z_{\mu-1}$ with $Z_1 = 1$.

For calculations of $V(\alpha+\beta,\gamma \mid f+g+M,h)$ a computational scheme may be derived from (28)

(31) $$V(\alpha+\beta,\gamma \mid f+g+M,h) = \sum_{\nu=1}^{N}{}' v_\nu$$

where $v_\nu = \frac{(\alpha+\beta)}{(\alpha+\beta+\gamma)} \cdot \frac{(f+g+h+M+\nu)}{(f+g+M+\nu)} v_{\nu-1}$ with $v_0 = \frac{A(\alpha+\beta+\gamma \mid f+g+h+M)}{(\alpha+\beta)}$,

V. CONVERGENCE PROPERTIES

$W(\alpha\beta\gamma|pqh)$. The scheme for calculation of W with $h<0$, defined in (30) includes three infinite sums and the rate of convergence for each of them is essential.

In actual calculations α, β and γ will be of roughly the same order of magnitude and we will limit our discussions of the convergence properties to this case.

The factors containing μ or ν in the recursion formulas for X_μ, η_μ and S_ν, converge to unity and the latter may be approximated as follows

$$X_\mu \approx \left(\frac{\alpha}{\alpha+\beta}\right)^\mu$$

(32)
$$\eta_\mu \approx \mu!\left(\frac{\alpha+\beta}{\alpha+\beta+\gamma}\right)^\mu$$

$$S_\nu \approx \left(\frac{\alpha+\beta}{\alpha+\beta+\gamma}\right)^\nu$$

Obviously the convergence for X_μ and S_ν is faster than for η_μ, and consequently $\sum_{\mu=2}^{M} \eta_\mu$ in (30) is the critical part.

Actually Σ_0 is zero for M infinite, and (30) may be replaced by

(33)
$$W(\alpha\beta\gamma|pqh) \approx W_0 \sum_{\mu=2}^{M} \eta_\mu$$

The number of multiplications (or divisions) needed to calculate W by (30) and by (33) is respectively

(34)
$$m_1 = 10M + 3N \qquad \text{and} \qquad m_2 = 6M.$$

Rather than giving an extensive theoretical treatment of the convergence properties of W, we have chosen to exemplify its behavior by calculating $W(\alpha\beta\gamma|00-1)$ for some typical values for (α,β,γ). As seen from formulas (27) and (31) the choice of $(\xi,\eta,h)=(0,0,-1)$ represents some of the worst convergence properties possible. In table I we have tabulated the number of significant decimal figures d of W, calculated by (30), as a function of M and N. Table II shows the number of significant figures d' as a function of M, when W is calculated by (33).

From (34) and Tables I and II algorithms may be derived for the choice of M and N. In principle one could even give M and N as explicit functions of the arguments $\alpha,\beta,\gamma,\xi,\eta,h$ and the desired number of significant figures d.

$I(\alpha\beta\gamma|\rho\eta s|11-1)$ As an example of the behavior of W with negative h, we have chosen to treat $I^{000}_{\cdots}$ for $(\lambda,\mu,\nu)=(1,1,-1)$. The explicit formula for calculation of the integral is given in (23), but to simplify the discussion we rewrite this equation as

(35) $$I(\alpha\beta\gamma|\rho\eta s|11-1)=D_0+\sum_{k=1}^{K}D_k$$

where K is in principle infinite, and the definitions of D_0 and D_k are obvious.

For each of the fourteen W's appearing in D_k, we have the relation

(36) $$\xi+\eta+h=\rho+\eta+s+7$$

When k is large enough all the W's will have $k<0$ and W_0 in (30) will be approximately constant. Further $j+q+k$ is obviously independent of k, so even under the summation over k the variation in W_0 will be represented by the factor $(j+1)^{-1}$ and this variation is very small for large k. In fact this is the main variation for each of the W's. The approximate constancy of the W's, shows that the D_k behave like k^{-4}, and this gives a good estimation of the convergence properties of $\sum_{k=1}^{\infty} D_k$.

Table I

The number of significant figures, $d(M,N)$ in $W(\alpha,\beta,\gamma|0,0,-1)$ calculated by (30).

a) $\alpha,\beta,\gamma = 2,2,2$

M \ N	10	20	30	40	50	60
10	4	5	5	5	5	5
20	6	8	10	10	10	10
30	8	10	11	13	15	15
40	10	11	13	15	15	15
50	11	13	15	15	15	15
60	13	15	15	15	15	15

b) $\alpha,\beta,\gamma = 1,1,4$

M \ N	5	10	15	20
5	4	5	5	5
10	7	9	9	9
15	10	12	13	13
20	12	15	15	15

c) $\alpha,\beta,\gamma = 1,4,1$

M \ N	20	40	60	80	100
20	4	6	7	9	11
40	6	7	9	11	12
60	7	9	11	12	14
80	9	11	12	14	15
100	11	12	14	15	15

d) $\alpha,\beta,\gamma = 4,1,1$

M \ N	20	40	60	80	100
20	3	4	4	4	4
40	5	7	7	8	8
60	7	8	10	11	11
80	8	10	12	13	15
100	10	12	13	15	15

We have chosen to carry 16 decimal figures (Fortran double precision) in our calculations, because in combining the $I:s$ to matrix elements, necessary in the variational calculation, cancellation of significant figures will occur in some cases (e.g. when the radial parts of the orbitals are Laguerre functions).

Table II

The number of significant figures $d'(M)$, in $W(\alpha,\beta,\gamma|0,0,-1)$ calculated by (33).

M \ (α,β,γ)	(4,1,1)	(1,4,1)	(2,2,2)	(1,1,4)
5	0	0	1	2
10	0	1	2	5
15	1	2	3	7
20	1	2	4	10
25	2	3	5	12
30	2	3	6	15
40	3	4	8	
50	4	5	10	
60	5	6	11	
70	6	6	13	
80	7	7	15	
100	8	9		
120	10	11		
140	12	12		
160	13	14		
180	14	14		
200	14	14		

APPENDIX

As an example we will discuss the integrals produced by a correlated wave function for a three electron atomic problem. An adequate trial wave function for a doublet state can be written

(A1) $$\Psi(1,2,3) = \mathcal{A}\,\Psi_A(1,2)\Psi_B(3)$$

where $$\Psi_A(1,2) = \Phi_A(\underline{r}_1,\underline{r}_2)\{\alpha(1)\beta(2)-\beta(1)\alpha(2)\}$$

and $$\Psi_B(3) = \Phi_B(\underline{r}_3)\alpha(3)$$

After integration over the spin variables the average value of the Hamiltonian becomes

$$\langle H\rangle_{AV} = \frac{\langle\Phi_A(1,2)\Phi_B(3)\,|\,H(1-P_{23})\,|\,\Phi_A(1,2)\Phi_B(3)\rangle}{\langle\Phi_A(1,2)\Phi_B(3)\,|\,(1-P_{23})\,|\,\Phi_A(1,2)\Phi_B(3)\rangle}$$

where P_{23} is the permutation operation that interchanges the electron coordinates 2 and 3. For an S-state we may choose the space functions

(A2) $$\Phi_A(1,2) = e^{-a(r_1+r_2)}(1+c\,r_{12})$$

and $$\Phi_B(3) = e^{-b r_3}\,r_3$$

The only part of the Hamiltonian, that involves calculation of an integral $I(\alpha\beta\gamma|\rho\sigma\tau|\lambda\mu\nu)$ with λ, μ and ν all $\neq 0$ is $\frac{1}{r_{23}}$

The evaluation of

$$\left\langle \frac{1}{r_{23}} \right\rangle_{AV} = \frac{1}{\Delta}\Big\{ I(2b,2a,2a|200|-100) + 2c\, I(2a,2a,2b|002|1-10)$$

(A3)
$$+ c^2 I(2a,2a,2b|002|2-10) - I(a+b,a+b,2a|110|-100)$$

$$-2c\, I(a+b,a+b,2a|110|-110) - c^2 I(2a,a+b,a+b|011|11-1)\Big\}$$

where

$$\Delta = I(2a,2a,2b|002|000) + 2c\, I(2a,2a,2b|002|100)$$

$$+ c^2 I(2a,2a,2b|002|200) - I(2a,a+b,a+b|011|000)$$

$$-2c\, I(2a,a+b,a+b|011|100) - c^2 I(2a,a+b,a+b|011|110)$$

will serve to demonstrate the convergence of the infinite series in (23) for calculation of $I(\alpha\beta|\gamma\delta s|11-1)$ and also the importance of this term in the average value. For the Li-atom $a=2.56$, $b=1.4$ and $c=0.36$ would give a fair approximation[4] to the ground state wave function.

In Table III we list D_0 and the first fifteen D_k in the infinite sum, that appears in the definition (35) and (23) for $I(2a,a+b,a+b|011|11-1)$. The observed convergence for the series is actually better than for $\sum_{k=1}^{\infty} k^{-4}$ and it is justified to conclude that the remainder in general is

$$\sum_{k=K+1}^{\infty} D_k < \frac{1}{3} K D_K$$

which in our example means that we have eight significant figures in I.

The W^A appearing in each D_{λ} were calculated by (30) with $M=N=40$, which according to Table I gives eleven or twelve significant figures, and as no appreciable cancellations occur in the formation of each D_{λ} this does not influence the accuracy of I.

Table IV. lists the integrals I and we like to point out the the above mentioned integral $I(2a,a+b,a+b|011|11-1)$ may definitely not be neglected in the calculation of the average value.

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Table III

D_k, for k = 0, 1, 2, ... 12, as defined by (23) and (35) for the integral $I(5.72, 4.26, 4.26 \mid 0\ 1\ 1 \mid 1\ 1\ -1)$.*

$$D_0 = 0.358\ 027\ 6958 \cdot 10^{-5}$$
$$D_1 = 0.004\ 913\ 4950 \cdot 10^{-5}$$
$$D_2 = 0.000\ 046\ 7536 \cdot 10^{-5}$$
$$D_3 = 0.000\ 002\ 9199 \cdot 10^{-5}$$
$$D_4 = 0.000\ 000\ 3819 \cdot 10^{-5}$$
$$D_5 = 0.000\ 000\ 0759 \cdot 10^{-5}$$
$$D_6 = 0.000\ 000\ 0199 \cdot 10^{-5}$$
$$D_7 = 0.000\ 000\ 0063 \cdot 10^{-5}$$
$$D_8 = 0.000\ 000\ 0023 \cdot 10^{-5}$$
$$D_9 = 0.000\ 000\ 0010 \cdot 10^{-5}$$
$$D_{10} = 0.000\ 000\ 0004 \cdot 10^{-5}$$
$$D_{11} = 0.000\ 000\ 0002 \cdot 10^{-5}$$
$$D_{12} = 0.000\ 000\ 0001 \cdot 10^{-5}$$

and consequently

$$I(5.72, 4.26, 4.26 \mid 0\ 1\ 1 \mid 1\ 1\ -1) = 0.362\ 991\ 35 \cdot 10^{-5}\ .$$

* Errata

Formulas (23) and (35) for calculation of $I^{000}_{000}(\alpha\beta\gamma \mid pqs \mid 1\ 1\ -1)$ are not correct. The term

$$D_0 = \tfrac{1}{5}\left[W(\alpha\beta\gamma \mid p+6, q+1, s) + W(\beta\alpha\gamma \mid q+4, p+3, s) + W(\gamma\beta\alpha \mid s+4, q+3, p) \right.$$
$$\left. + W(\alpha\gamma\beta \mid p+6, s+1, q) + W(\beta\gamma\alpha \mid q+4, s+3, p) + W(\gamma\alpha\beta \mid s+4, p+3, q) \right]$$

should be deleted and the summation $\sum_{k=1}^{\infty}$ replaced by $\sum_{k=0}^{\infty}$. The correct formulas were used for the calculations reported in Tables III and IV.

Table IV

Integrals $I(\alpha, \beta, \gamma | p, q, s | \lambda, \mu, \nu)$ appearing in formula (A3).

α	β	γ	pqs	λ	μ	ν	I
2.8	5.72	5.72	200	-1	0	0	$1.084\,350\,608 \cdot 10^{-5}$
5.72	5.72	2.8	002	1	-1	0	$0.819\,094\,061 \cdot 10^{-5}$
5.72	5.72	2.8	002	2	-1	0	$0.774\,239\,416 \cdot 10^{-5}$
4.26	4.26	5.72	110	-1	0	0	$0.346\,281\,001 \cdot 10^{-5}$
4.26	4.26	5.72	110	-1	1	0	$0.343\,730\,385 \cdot 10^{-5}$
5.72	4.26	4.26	011	1	1	-1	$0.362\,991\,353 \cdot 10^{-5}$
5.72	5.72	2.8	002	0	0	0	$1.592\,593\,371 \cdot 10^{-5}$
5.72	5.72	2.8	002	1	0	0	$1.218\,111\,188 \cdot 10^{-5}$
5.72	5.72	2.8	002	2	0	0	$1.168\,218\,522 \cdot 10^{-5}$
5.72	4.26	4.26	011	0	0	0	$0.354\,705\,251 \cdot 10^{-5}$
5.72	4.26	4.26	011	1	0	0	$0.387\,786\,480 \cdot 10^{-5}$
5.72	4.26	4.26	011	1	1	0	$0.433\,603\,504 \cdot 10^{-5}$

$$\Delta = 1.930\,928\,02 \cdot 10^{-5}$$

$$\left\langle \frac{1}{r_{23}} \right\rangle_{AV} = 0.587\,090\,36$$

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